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Final Report

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UV Raman and Fluorescence for Multi-Species Measurement in Hydrocarbon-Fueled
High-Speed Propulsion

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Introduction

This report documents work performed through the NASA Graduate Student Researchers Program, Grant No. NGT3-52316. Research performed included investigation of two-line fluorescence imaging of OH for temperature measurement and an investigation of negative flame speeds for modeling of premixed turbulent flames. The laboratory work and initial analysis of the fluorescence imaging was performed at NASA Glen Research Center with follow up analysis at Vanderbilt University. The negative flame speed investigation was performed using an opposed jet flow simulation program at Vanderbilt University. The fluorescence imaging work is presented first followed by the negative flame speed investigation.

Two-Line Fluorescence Imaging of OH for Temperature Measurement

In combustion flows, two-dimensional temperature fields can provide important information. The two-dimensional temperature field can be used as a visualization of the flow field. The field can also be used to isolate regions of burned and unburned gases as well as give an indication of the fuel/air mixing.

Two-line planar laser-induced fluorescence (PLIF) of OH can be used to create the two-dimensional temperature field. The number of photoelectrons, N , collected from a fluorescence image is given by¹

$$N = \eta V_c n_a f(T) B E g(\nu) F$$

where

- η = overall efficiency of collection optics and detector,
- V_c = measurement volume,
- n_a = absorbing species number density,
- $f(T)$ = fractional Boltzmann population,
- B = Einstein coefficient for absorption,

E = laser energy fluence,
g(v) = spectral overlap integral, and
F = fluorescence yield A/(A + Q).

A ratio of two PLIF images (1 and 2) excited from different lower states give

$$\frac{N_1}{N_2} = C \frac{f_1(T)B_1E_1g_1F_1}{f_2(T)B_2E_2g_2F_2}$$

where C is a constant dependent on the relative optical and detector efficiencies. Assuming only Boltzmann population fractions are temperature dependent, the ratio of the images become

$$\frac{N_1}{N_2} = C \frac{E_1}{E_2} \exp(-\Delta e_{12}/kT).$$

The term Δe_{12} is the energy difference between the two pumped lower energy levels. All the constant coefficients are included in the single calibration constant, C. The temperature of the flame is therefore given by

$$T = \frac{-\Delta e_{12}}{k \ln \left[\frac{N_1 E_2}{C N_2 E_1} \right]}.$$

This technique was demonstrated in the post flame zone of a small Hencken burner at atmospheric conditions. This technique is investigated for application in a high-pressure combustor at NASA Glen Research Center.

The experimental setup is shown in Figure 1. Although two lasers are shown, only one laser was used in the initial investigation. The beam from a tunable dye laser is formed into a sheet approximately 1.5 cm in height and directed over a 2.54 cm square co-flow Hencken burner burning methane-air. The fluorescence images are recorded on Princeton Instruments ICCD cameras. Rayleigh scattering and background scattering were reduced by using a UG11 filter and a 313 nm (10 nm FWHM) band pass filter. A quartz window was placed in the path of the beam to reflect a small portion of the beam into a Star Tech BIP-5100 series beam profiler. The profiler was placed so the distance from the window to the beam profiler and the burner were the same.

A theoretical determination of the temperature profile was given above. However, to determine the temperature distribution in a flame, experimental conditions must be addressed. For a true fluorescence distribution, background, laser beam fluctuations, beam profile, and detector responses must be accounted for. Each fluorescence image must be corrected for each of these experimental conditions by the following graphical expression:

$$\text{Corrected Image} = \left\{ \frac{(\text{PLIF Raw Image} - \text{Background})/\text{PLIF ICCD response}}{(\text{Beam Profile} - \text{Background})/\text{Beam Profile ICCD response}} \right\}.$$

The image is corrected by the beam profile because the profile is Gaussian and the profile may vary with wavelength. The image must also be corrected by the camera response as it will also vary with wavelength.

The temperature distribution can now be determined by

$$\text{Ratio} = \frac{\text{Corrected Image 1}}{\text{Corrected Image 2}}$$

and

$$T = \frac{-\Delta e_{12}}{k \ln[C \text{ Ratio}]}$$

where C is a calibration constant. For the OH molecule the $A^2\Sigma^+ \leftarrow X^2\Pi$ transition is used. Figure 2 shows the energy level diagram of OH for the $A^2\Sigma^+ \leftarrow X^2\Pi$ transition. Also shown in the figure are possible line pairs for the temperature measurement. In determining the lines to pump and the pairs to use, several factors were considered. The technique is to be applied in an environment where temperature measurements of 1400-2100 K are desired. Therefore, population of the energy levels must be examined. A Boltzmann model was used to model the energy level populations. The lines also needed to be spectrally isolated from other lines. This ensures that only the chosen line is excited. Transitions must also be selected that do not cause beam attenuation in the flame.

The two-line PLIF temperature measurement was applied to a small Hencken burner at atmospheric pressure. The laboratory experiment revealed several concerns that need to be addressed before the technique can be applied in a high-pressure combustor. First, alignment must be investigated further. It is very crucial that the beam travels the same path when the wavelength is changed. This is very difficult to achieve since the pelin brocca prism in the doubler redirects the beam when the wavelength is changed. The response of the ICCDs with wavelength must also be studied.

Once the system has been tested in the atmospheric laboratory, new considerations must be addressed in the high-pressure combustor environment. In selecting the line pair, laser attenuation must be revisited. Also, pressure and collisional broadening effects that are not present at atmospheric conditions must be considered. Soot formation on the combustor windows is fuel injector dependent and will cause problems in receiving the fluorescence signals. Although the high-pressure combustor will be operating in lean conditions, there will be pockets of rich regions. These regions will cause PAH interferences.

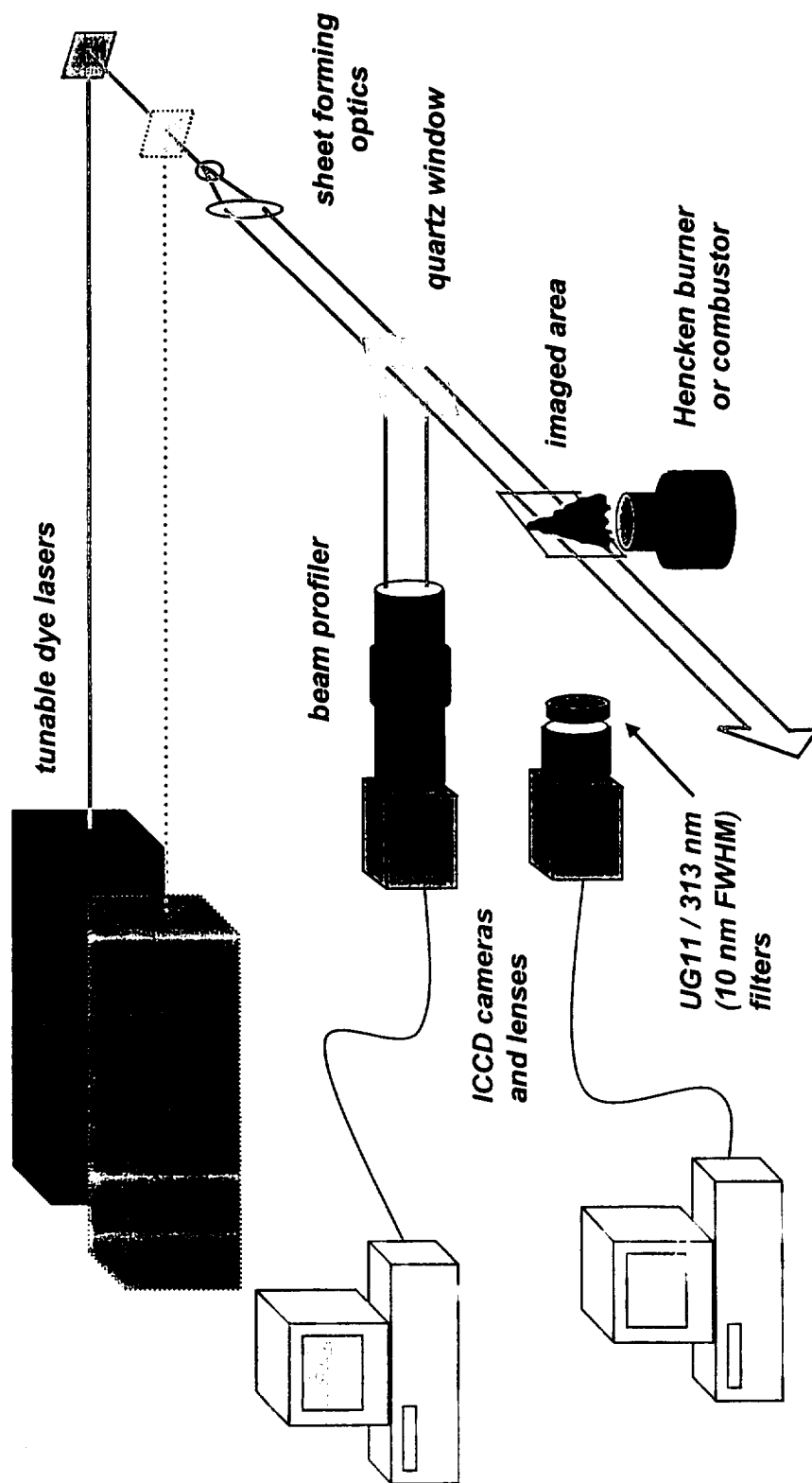


Figure 1 Two-line PLIF experimental setup.

Possible line pairs for the $A^2\Sigma^+ \rightarrow X^2\Pi$ transition

$R_1(9) - 281.363 \text{ nm}$	$R_1(12) - 281.967 \text{ nm}$
$R_1(10) - 281.522$	$Q_1(11) - 284.765$
$R_2(10) - 281.853$	$O_2(5) - 285.500$
$R_1(12) - 281.967$	$Q_1(13) - 285.785$
$R_2(11) - 282.035$	$P_1(7) - 284.992$
$R_2(11) - 282.035$	$Q_2(12) - 285.533$
$Q_2(9) - 284.250$	$O_2(5) - 285.500$
$Q_1(10) - 284.316$	$O_2(5) - 285.500$
$P_1(7) - 284.992$	$Q_2(11) - 285.061$

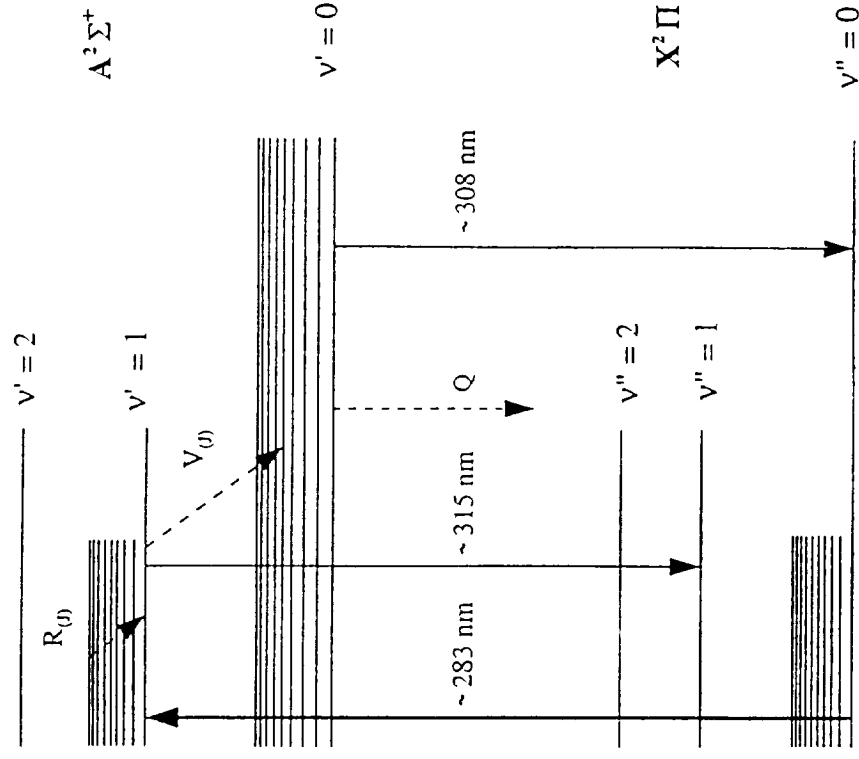


Figure 2 Energy level diagram of OH and possible line pairs.

Negative Flame Speed Investigation

The turbulent flames in lean premixed (LP) gas turbine combustors are stabilized by recirculation. The hot products of combustion in the recirculation zone essentially support reaction zones of weak lean reactants. The structure of these reaction zones is compared to laminar flamelet models. The flamelet model is comprised of a library of thin laminar flamelets over a range of strain rates. An opposed jet flame configuration is used for modeling a stretched laminar flamelet. Here a jet of cold ($T = 300$ K) LP propane/air at an equivalence ratio of 0.6 opposes a jet of hot ($T = 1700$ K) equilibrium products of propane/air combustion at the same equivalence ratio. This configuration is a realistic simulation of the flame in the recirculation zones of LP gas turbines.

The premixed flame calculations for the opposed flow geometry at various strain rates are shown in Fig. 3. The flame is calculated with the Chemkin III family of computer codes.²⁻³ The flame location and the reaction zone are defined by the peak OH concentration. At low strain rates ($a = 200$ s⁻¹), the flame resides on the unburnt gas side of the stagnation plane: evidenced from the peak OH and CO concentrations. At low strain rates ($a < \sim 500$ s⁻¹), the flame is self-propagating because of the diffusion of heat and radicals from the reaction zone to the preheat zone of the premixed flame. In self-propagating premixed flames, the combustion scalars (species and temperature) are insensitive to strain rate and the radical concentrations are high. The peak OH concentrations in the figure are ~ 2250 ppm.

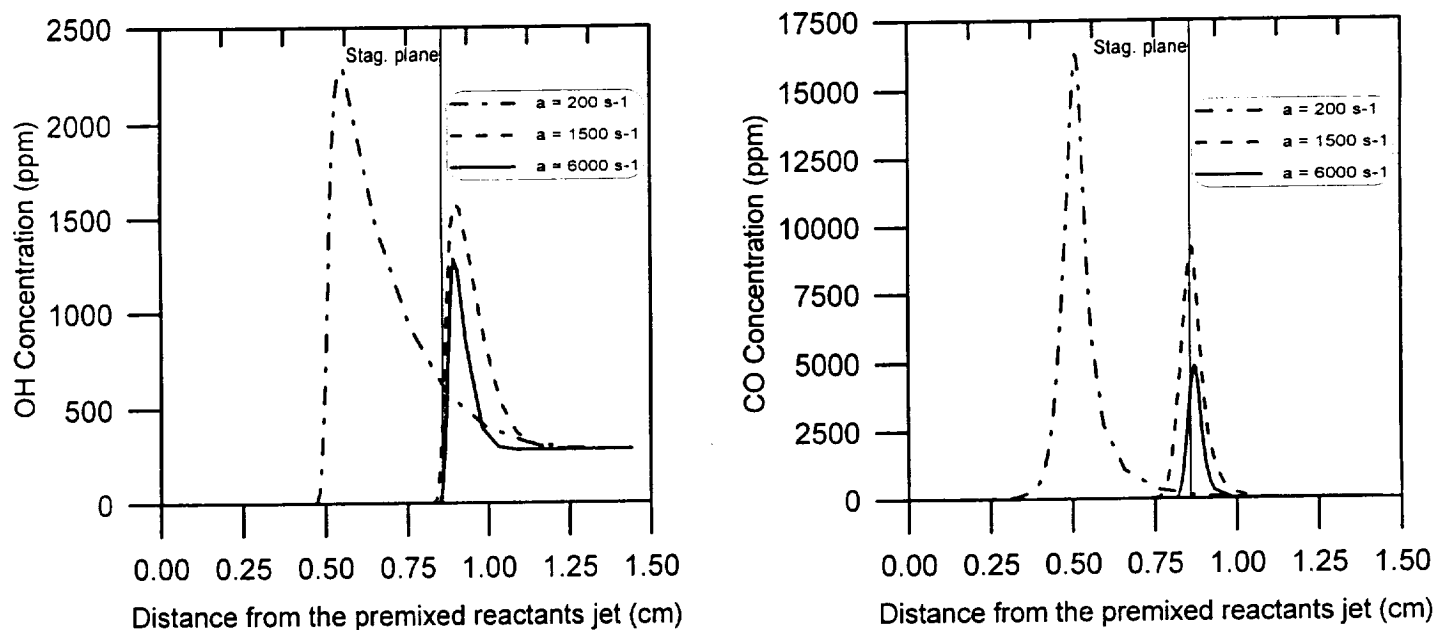


Figure 3. Calculated concentrations of OH and CO in opposed jet flames at various strain rates. The opposed flow flame configuration used for modeling was a jet of cold ($T = 300$ K) LP propane/air at an equivalence ratio of 0.6 opposed by hot ($T = 1700$ K) equilibrium products of propane/air combustion at the same equivalence ratio.

However, previous measurements⁴ in bluff-body stabilized turbulent LP methane flames have revealed that the peak OH concentrations in the recirculation zone are only ~700 ppm. Such low radical concentrations are possible only in a flame that is not freely propagating. In an opposed jet configuration, a non-freely propagating flame can be obtained by increasing the strain rate considerably. At high strain rates ($a > \sim 500 \text{ s}^{-1}$), the flame is pushed across the stagnation plane from the unburnt gas side to the burnt gas (hot products) side as seen in the figure. These flames are not self-propagating and are termed as flames with negative displacement speed.

In premixed combustion, displacement speed or flame speed (S_L) is defined as the propagation of flame with respect to the local gas velocity. In the opposed jet calculations, the flame is stationary in the laboratory frame. So if the flame resides on the burnt gas side of the stagnation plane (as the high strain flames of the figure), the displacement speed is negative. The concept of negative flame speed for premixed combustion is elucidated with the transport equation:

$$\underbrace{\rho_u S_L \frac{dY_i}{dx}}_{\text{Convection}} + \underbrace{\frac{d}{dx}(\rho V_i)}_{\text{Diffusion}} = \underbrace{\dot{\omega}_i}_{\text{Reaction}}$$

where ρ is the density, S_L is the laminar flame speed, Y is the mass fraction, V is the diffusion velocity, $\dot{\omega}$ is the production rate, and the subscripts u and i refer to the unburnt mixture state and species i respectively. From the above equation, it is clear that a negative S_L implies that diffusion exceeds reaction locally, to counter adverse (negative S_L) convective fluxes. Flames with negative displacement speed are not self-sustaining and the radicals are sensitive to strain rate. They are sustained by the presence of the hot product stream that provides heat and radicals to the flame through diffusion and molecular mixing. So premixed flames with negative displacement speed exhibit diffusion or mixing controlled flame behavior. This is similar to non-premixed flames where fuel/air mixing controls the rate of combustion. In “negative speed” flames, the rate of combustion is controlled by the rate of mixing of weak lean reactants with hot products. This is a new and interesting concept that would influence the combustion parameters such as the flame structure, topology, heat release, fuel consumption and the pollutant formation. Hence, conventional models currently in use for computing the recirculation stabilized lean premixed turbulent flames need to be modified to account for this mixing controlled burning in lean premixed combustion supported by recirculation.

Summary

A two-line PLIF of OH has been investigated for application in a high-pressure combustor. The technique was applied in a Hencken burner at atmospheric conditions. The laboratory experiment revealed several concerns that need to be addressed before the technique can be applied in a high-pressure combustor. However, initial results indicate that two-line PLIF of OH can be used for temperature measurement in lean conditions.

Lean premixed strained opposed jet flames are computationally investigated as a model of lean premixed turbulent combustion. The effect of strain rate on lean premixed flames ($\phi=0.6$) is investigated for a jet of lean premixed propane reactants opposing hot products. At low strain rates, the minor species concentrations (e.g. OH and CO) are independent of strain rate. The peak values of minor species are unchanged with increasing strain rate. Under these conditions, the lean premixed flame is self-propagating and not affected by strain rate.

At high strain rates, the lean premixed reactants are pushed into the hot products. The flame is controlled by mixing of weak reactants with the hot products. This is a so-called "negative flame speed" flame. Under these conditions, the minor species concentrations are greatly affected by the strain rate. Peak concentrations of CO and OH are greatly reduced. The calculated concentrations are consistent with previous measurements in lean premixed turbulent flames.⁴ The calculations suggest that mixing controlled flames are important in lean premixed combustion at high turbulence levels.

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